

2-Butanone oxime
96-29-7 | DTXSID1021821

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.12e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.71e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

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2-Butanone oxime

Measured: 1.15

Predicted: 9.12e-01

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2-Methyl-2-butenal

Measured: 2.97e-01

Predicted: 4.88e-01

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2-Pentanone

Measured: 4.99e-01

Predicted: 4.58e-01

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2-Methylpropanal

Measured: 1.23

Predicted: 1.31

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Butyraldehyde

Measured: 9.85e-01

Predicted: 5.88e-01